Laboratory Name: Brookhaven National Laboratory
B&R Code: KC0201030

FWP and possible subtask under FWP: Superconducting Materials

FWP Number: MA-012-MABA

Program Scope: This program studies the basic relationships between nanoscale structures and macroscopic properties of superconductors, providing the understanding of the fundamental physics and materials science required for their practical utilization. High temperature superconducting (HTS) cuprates, alloyed MgB_2, and superconductor / magnet heterostructures are systems receiving emphasis.

Major Program Achievements (over duration of support):
1) Using magneto-optical imaging coupled with optical and atomic force microscopy (AFM), we observed enhanced flux pinning in superconducting $YBa_2Cu_3O_{7-\delta}$ (YBCO) films, which resulted in ~ 30% increase in critical current density J_c. The origin of enhanced pinning was nanometer-scale substrate surface roughness, which was created by surface reconstruction in a twin-rich region of the film substrates. The enhancement was absent in an adjacent twin-free region of the same film on the same substrate.

2) Magneto-optical imaging techniques coupled with ac (hysteresis) loss measurements were used to investigate the magnetic interaction between vortices in YBCO films on magnetic substrates. It was found that magnetic coupling between these components reduced the ac losses by making the curvature of flux lines less in superconducting films.

3) Studies of structure, heat capacity, and transmission electron microscopy with electron energy loss spectroscopy were coordinated to probe the changes in superconductivity in MgB_2 when the Mg atoms are progressively replaced by Al. We obtained the first direct evidence for the filling of the hole states in the planar σ band, which are crucial for the high critical temperature in pure MgB_2, by the extra electrons donated by Al. Yet, other property measurements indicated that superconductivity was not destroyed when there was sufficient Al to fill all of the hole states, but it persisted to much higher levels of Al doping. Using a two-band model of superconductivity, fits to the heat capacity data indicated that it is the π band that survives in the heavily doped regime, which is an inversion of the hierarchy of the bands in pure MgB_2.

4) Analyses of x-ray diffraction patterns of Al- and C-alloyed MgB_2 showed that typical reactions that produce good samples of pure MgB_2 do not produce homogeneously alloyed samples. The inhomogeneities can skew property trends as a function of the intended composition. However, by referencing property trends to the x-ray diffraction data, more uniform behavior was observed, suggesting that the effects of inhomogeneities are mitigated and the underlying physics can more clearly be assessed.

Program Impact: Results (1) and (2) suggest that incorporation of nanoscale or magnetic materials near the superconductor can enhance the critical current and reduce the ac loss in HTS coated conductors, which will be the next generation of superconductors for electricity applications. Results (3) explain why the critical temperature falls with dopant concentration. Also, since π-band superconductivity occurs in intercalated graphite compounds with the same basic structure. Result (3) suggests that superconductivity in MgB_2 is not unique; rather it is an extraordinary example in a broader class of materials made possible by manipulation of the position of the σ band.

Interactions: Condensed Matter Physics and Materials Science Dept., CFN, SUNY at Stony Brook (P. Stevens, S. Sampath and R. Gambino), Penn State University (X. X. Xi), Los Alamos National Laboratory (L. Civale and S. Foltyn), GM R&D Lab (J. Yang), Specialty Materials Inc. (J. Marzik and A. Kumnik), Wisconsin (D. Larbalestier), Ames Laboratory (D. Finnemore and P. Canfield), Arizona State University (J. Rowell and N. Newmann), Superconducting Technologies Inc. (B. Moeckly)

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
Z. Ye (Advisor: Q. Li) – SUNY President Award for Outstanding Ph. D Graduates, 17 invited talks

Personnel Commitments for FY2005 to Nearest +/-10%: Q. Li (Co-PI) 100%, L. Cooley(Co-PI) 50%, and A. Moodenbaugh 30%, Z. Ye (Grad. student) 100%

Authorized Budget (BA) for FY03, FY04, FY05:
FY03 BA - $974K **FY04 BA** - $974K **FY05 BA** - $729K

Laboratory Name: Brookhaven National Laboratory
B&R Code: KC0201010

FWP and/or subtask Title under FWP: Studies of Nanoscale Structure and Structural Defects in Advanced Materials

FWP Number: MA-015-MACA

Program Scope:
The goal of this program is to study property sensitive nanoscale structure and defects in technologically-important materials such as superconductors, magnets, and other functional materials. Advanced quantitative electron microscopy techniques, such as coherent diffraction, atomic imaging, column-by-column spectroscopy, and phase retrieval methods including electron holography are developed and employed to study material behaviors. Computer simulations and theoretical modeling are carried out to aid the interpretation of experimental data. Fabrication of thin films with tailored microstructure and nano-assemblies to understand materials' electronic and magnetic behaviors is also incorporated.

Major Program Achievements (FY2005):
(1) Fabrication of Permalloy elliptical elements with different aspect ratios and frustrated disk arrays to study magnetic dynamics and switching behavior; (2) Development of the theoretical framework for magnetostatic shape anisotropy and demagnetization effects that were observed with electron phase microscopy experiments; (3) Quantitative measurement of interfacial displacement and local lattice parameter at the $YBa_2Cu_3O_7$ twin boundaries and grain boundaries using the geometrical phase analysis method; (4) Combined study of the electronic structure of $CaCu_3Ti_4O_{12}$ single crystal using coherent electron diffraction (PARODI method), synchrotron x-ray diffraction, EXAFS and DFT calculations to understand the material's gigantic dielectric behavior; (5) Understanding electron doping and straining effects and the two-band superconductivity in MgB_2 using high-resolution EELS and DFT; (6) Analysis of beam damage and dose optimization for imaging of single molecules with aberration (Cs) corrected microscopes. Revealing the cooperative doping effect of Ca at the $YBa_2Cu_3O_7$ grain boundaries for increased interfacial critical current density; proposing how Tc might be raised via straining MgB_2 using first-principle analysis; completing the magnetic phase diagrams of nano-rings that provide essential information to MRAM developers and manufacturers.

Program Impact: The impact of this work is the development of advanced imaging techniques that can be broadly applied to quantitatively characterize a variety of materials and their behavior. Applications to high Tc superconductor and magnetic materials are demonstrated.

Interactions: Internal—Superconducting and magnetic materials group, Neutron scattering group, Synchrotron x-ray diffraction group, Solid-state theory group; Center for data intensive computing, and Biology STEM group. External—Columbia University; Stony Brook University; Carnegie Mellon University; Yale University; University of Alberta, Canada; University of Oslo, Norway; and University of Bologna, Italy.

Recognitions, Honors and Awards (at least in some part attributable to support under this program):
Y. Zhu – Distinguished Science and Technology Award, BNL (2003); Program Committees and symposium co-organizer, MSA (2002, 2004), MRS (2005); NSF national panel for Major Instrumentation for Materials Research, (2002); Editorial Board of *MICRON*, Adjunct Professor at Dept. of Applied Physics and Mathematics, Columbia University; Dept. of Physics and Materials Science, Stony Brook University; R. Klie – BNL Goldhabor Fellow (2002-2005), M. Beleggia – Prize "Carla Milanesi", Italian Society of Electron Microscopy for the outstanding contributed paper at the MCEM5th conference (2002), J. Lau et al, Best poster Award, 49th Mag, Mag. Mat. conference (2004). J. Lau, National Research Council Postdoc Fellow (2005). 31 invited talks in the last three years at major conferences excluding institution seminars.

Personnel Commitments for FY2005 to Nearest +/- 10%: Y.Zhu (80%), L.Wu (100%), V.Volkov (100%), M.Schofield (100%), J.Bording (100%), M.Beleggia (100%), R.Klie (80%), J. Lau (100%) and J. Zheng (100%).

Authorized Budget (BA):
FY03 BA - $1,350K **FY04 BA -** $1,532K **FY05 BA -** $1,598K

Laboratory Name: Brookhaven National Laboratory
B&R Code: KC0203010

FWP and possible subtask under FWP: Biology-inspired programmable assembly of functional nano-structures.

FWP Number:
MA-114-MAAA

Program Scope:

An understanding of the interplay between selective biological factors and non-selective physical factors in hybrid systems is the key question of bio-programmable assembling, and this is the central goal of our research program. In addition, underlying all work in bio-assembly is the need for a broader library of biological tools that provide the required selectivity of interaction, and methods for linking the biological elements to the inorganic nano-materials. Our research strategy combines an exploration of the microscopic structure of nano scale objects with a range of methods for the assembly of such systems, including both biochemical and physiochemical approaches.

Major Program Achievements (over duration of support):

Developed method for functionalization of carboxyl terminated surfaces with high density monolayer of single and double stranded oligonucleotides. Obtained the first results on stabilization of the DNA-particle suspension through: (i) decreasing ionic strength of the solution that increases the electrostatic repulsion between negatively charged backbones of oligonucleotides; (ii) balancing the number of hybridizations per pair of particles. Our preliminary results show that dynamic range of interactions can be tuned in such a way that the phase of the system can be varied from a nearly dispersed particles state or disordered particles aggregates to and close-packed particles assemblies.
Carried out a study of the interaction between DNA binding proteins, controlling heavy metal resistance in Ralstonia metallidurans, and their specific DNA binding domains. In order to functionalize DNA scaffolds with DNA we selected two DNA binding proteins, PbrR and ArsR, and examined the specificity of their binding to target DNA molecules. However, we first developed the protocols for the expression of soluble, functional forms of these two proteins, a prerequisite for this work. Once we obtained sufficient soluble and functional quantities of the two proteins we analyzed their binding to specific DNA fragments by gel retardation studies. Both proteins were found to specifically recognize their own DNA binding sequence. These two proteins will now be used to functionalize DNA coated particles and DNA scaffolds.

Program impact:

Understanding the assembling of nano-materials in ordered and pre-design structures will enable a broad array of applications in energy and environmental security.

Interactions:

Internal: BNL-Biology, BNL – MSD/CMP, BNL-Medical
External: AlUniversity of Michigan, University of Illinois, Stony Brook Univ.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):

Personnel Commitments for FY2005 to Nearest +/- 10%:

Oleg Gang (PI) 50%
Daniel van der Lelie (PI): 20% ??
Dmytro Nykypanchuk (postdoc) 70%

Authorized Budget (BA):

FY03 BA - $N/A **FY04 BA -** $N/A **FY05 BA -** $360K

Laboratory Name: Brookhaven National Laboratory
B&R Code: KC0202020

FWP and/or subtask Title under FWP: Fundamentals of Magnetic Nanomaterials

FWP Number: MA410 MABA

Program Scope:
The objective of this program is to attain an understanding of magnetic behavior of individual building blocks of materials and their synergies when combined into complex nanostructures leading to new functionalities that support selected missions of the DOE. Attention is focused on both intrinsic and extrinsic materials factors, especially as the size of the magnetic system progresses from the bulk to the nanoscale. Research goals are achieved by a combination of advanced non-equilibrium materials synthesis techniques, advanced probes (TEM, NSLS, force probe microscopies), magnetic measurement and theory to elucidate the factors underlying the magnetic response of magnetic nanomaterials, with the goal of controlling and tailoring the functional response to prescribed parameters.

Major Program Achievements (over duration of support):
Provided clear experimental and computational results that confirm formation of multi-grain "interaction domains" in nanocrystalline magnetic materials that significantly alters the nature of the magnetic reversal;

Demonstrated that interphase magnetic exchange is sensitive to the degree of interfacial epitaxy via studies of model exchange-spring bilayer samples of Co and $L1_0$-type CoPt, SmCo and Fe.

Demonstrated that magnetostructural transitions underlying functional responses (*i.e.*, colossal magnetoresistance effect, giant magnetocaloric effect; giant magnetic shape memory effect) in nanoscaled materials may be manipulated by external fields, including strain. In the course of these investigations we i) verified effects of extrinsic strain fields on the magnetostructural response of $Gd_5(Ge,Si)_4$ heterostructures that produced an overall reduction of magnetic field necessary to drive the transition; ii) confirmed a large reduction (> 100 K) in the magnetostructural transition of ferromagnetic MnBi nanorods.

Program impact:
Clarified the structural and magnetic factors controlling the technical magnetic response in nanocomposite ("exchange spring") magnets and thereby added to the knowledge base of advanced high-energy product magnet design. Demonstrated that the functional effect inherent in the magnetostructural transition may be manipulated in strain-temperature-field parameter space.

Interactions:
Ames Laboratory (rapidly-solidified NdFeB, bulk magnetic glasses and bulk exchange-spring systems), Carnegie Mellon University, Argonne National Laboratory (reversal studies in model magnetic bilayer systems); SUNY Stony Brook (nanostructured magnetocaloric & high-frequency materials); University of Western Australia (reversal studies in model magnetic bilayer systems); Magnequench Intern'l, Inc. (structure/property relationships in $Nd_2Fe_{14}B$-based nanocrystalline magnets); IEN Torino, Italy (understanding the magnetostructural response in magnetic shape memory materials).

Recognitions, Honors and Awards (at least partly attributable to support under this FWP): (FY05)
(L. H. Lewis): Steering Committee; NASA Nanotech2005 Conference; Invited participant, NNI Workshop on Neutron and X-ray Facilities for Nanoscience: June 15 – 17 2005; Exec. Committee APS Topical Group on Magnetism (GMAG); AdCom and Finance Chair, IEEE Magnetics Society; Exhibits Chair, Joint MMM/Intermag Meeting (2007); Patent revision: "Simple Magnetic Field Amplification for Functional Magnetic Materials" .

Personnel Commitments for FY2005 to Nearest +/- 10%:
L. H. Lewis (97%), D. O. Welch (12%), K. Sutter (10%); E. Baumberger (MS student)

Authorized Budget (BA) for FY03, FY04, FY05

FY03 BA $389 K **FY04 BA** $375 K **FY05 BA** $--- K

Laboratory Name: Brookhaven National Laboratory
B&R Code: KC0201050

FWP and possible subtask under FWP: Synthesis and Characterization of Individual Carbon and Perovskite Oxide Nanotubes
FWP Number: MA-507-MAAA

Program Scope: The proposed research will unite synthesis of carbon and perovskite oxide nanotube materials, characterization of individual nanotube material properties, and theoretical studies with a goal of correlation of well-characterized and reproducibly synthesized nanotube materials with new physical properties. These studies will directly address fundamental scientific issues in nanotube materials with potential for significant impact on future technologies.

Major Program Achievements (over duration of support):

- Developed near edge X-ray absorption fine structure (NEXAFS) spectroscopy as an analytical tool to qualitatively and quantitatively study degree of order and alignment in carbon nanotube samples. Specifically, developed NEXAFS as a very effective technique at (a) identifying the phases with boron nitride nanotubes with the potential of distinguishing between hexagonal BN and cubic BN, and (b) monitoring the presence of defects and degree of crystallinity in nanoscale samples.
- Single-crystalline, submicron-sized $Bi_2Fe_4O_9$ cubes of reproducible shape have been successfully prepared using a facile, large-scale solid-state reaction employing a molten salt technique in the presence of a nonionic surfactant. The role of surfactant as well as alterations in the molar ratio of Bi^{3+} to Fe^{3+} precursors have been examined under otherwise identical reaction conditions and correlated with the predictive formation of different shapes of $Bi_2Fe_4O_9$ products.
- A series of single-crystalline $Ca_{1-x}Sr_xTiO_3$ ($0 \leq x \leq 1$) perovskite nanoparticle samples of reproducible, tunable composition was prepared using a simple, readily scaleable solid-state reaction between metal oxalates and anatase TiO_2 in the presence of NaCl and a nonionic surfactant. Shapes of the generated $Ca_{1-x}Sr_xTiO_3$ nanoparticles alter from cubes to quasi-spheres with decreasing 'x' values.
- Developed sensitive spectroscopic tools to determine the electroluminescence emission spectra from individual carbon nanotubes in-situ at a probe station where simultaneous transport studies are performed. Developed techniques for structural determination of the nanotube under probe.

Program impact

- We have determined the surface orientation and the degree of order in carbon nanotube arrays grown on a substrate.
- In studies of boron nitride nanotubes we have shown that *h*-BN was present in graphite-like form. These nanotubes were found to be highly crystalline and have a low defect density.
- We have demonstrated new methods for production of nanoscale magnetic materials.
- Our progress in the ability to synthesize single-crystalline nanomaterials with controllable chemical composition and morphology contributes to the wider materials community goal of rationally exploiting their nanoscale chemical and physical properties.
- We have discovered new method of optical emission was induced from a single carbon nanotube when electrons and holes were simultaneously injected into the nanotube from opposite ends. We have also performed the first simultaneous spectroscopy and direct structural determination on same nanotube; this work increases our understanding of the chiral dependence of the metallic tube energy splitting.

Interactions:
Internal: Condensed Matter Physics and Materials Science Department, National Synchrotron Light Source.
External: State University of New York Stony Brook, Columbia University, IBM Yorktown Heights, NIST.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
S.S. Wong – National Science Foundation CAREER award (2004-2008). 15 Invited talks.

Personnel Commitments for FY2005 to Nearest +/- 10%:
S.S. Wong (50%); J. Misewich (25 %)

Authorized Budget (BA) for FY03, FY04, FY05:
FY03 BA - $120K **FY04 BA -** $440K **FY05 BA -** $422K

Laboratory Name: Brookhaven National Laboratory
B&R Code: KC0201030 + KC020706 + KC0201030

FWP: Molecular beam epitaxy and nano-structuring of perovskite oxide materials toward an understanding of strongly correlated systems.

FWP Number: MA-509-MACA
Subtask under FWP: Bulk Materials Synthesis and Characterization.
Subtask under FWP: Mechanisms of Metal-Environment Interactions. [former **FWP Number:** MA-010-MAEA]

Program Scope:
Molecular beam epitaxy: We have developed a unique molecular beam epitaxy synthesis technique to synthesize atomically perfect thin films, multilayers, and superlattices containing cuprate high-temperature superconductors (HTS) and other complex oxides. This in turn enables fabrication of HTS heterostructures nanowires and nanodots of unprecedented quality.
Bulk Materials Synthesis: Design, synthesis and characterization of new materials; discovery of new phenomena associated with correlated electron behavior and problems in superconductivity and magnetism.
Metal-Environment Interactions: Determinations of the dominant rate controlling processes operative accompanying metal oxide formation and dissolution.

Major Program Achievements (over duration of support):
Molecular beam epitaxy: The new MBE laboratory, including a clean room, has been set up. The MBE growth chamber is fully functional; the first superconducting and atomically smooth films have been synthesized already. We have built setups for measurement of resistivity, susceptibility, photo-conductivity, and photo-inducted absorption. We have acquired a high-magnification Olympus BX51 optical microscope, upgraded an AFM, and ordered a high-resolution 4-circle X-ray diffractometer. A custom setup for parallel (32-channel) measurements of R(T) and the Hall effect will be completed shortly.
Bulk Materials Synthesis: Discovered colossal magnetoresistance (CMR) effect in Co-doped $FeSb_2$. Synthesized high purity samples of heavy fermion superconductors and discovered unconventional multi-band superconductivity. Developed new high temperature flux and in-situ spinning crystal growth method.
Metal-Environment Interactions: Demonstrated unusual surface corrosion susceptibility of a metallic layer on Al alloys produced by thermal and /or mechanical treatments using novel optical methods.

Program impact: These unique samples enable challenging experiments that deepen our understanding of materials that are governed by correlated electrons, thus providing the scientific base for their optimization and usage. Of particular note is the discovery of a giant proximity effect in the high temperature superconductors, which is stimulating much research worldwide.

Interactions: Internal: TEM (Zhu), XRD (Hill), soft X-ray scattering (Thomas, Abbamonte), nanowires (Misewich), catalysis (Adzic), ARPES (Valla, Johnson), NSLS (Kao, Nelson), theory (Tsvelik, Ku), neutron scattering (Zaliznyak, Gardner), nanotubes (Wang), nanowires arrays (Li).
External: LANL (Taylor), NHMFL (Boebinger), Rutgers (Chabal), Wisconsin (Lagally), Columbia (Osgood), Boulder (Dessau), Akron (Djordjevic), Miami (Clayhold), Stony Brook (Gurvich), Princeton (Ong), Johns Hopkins (Broholm, Chien), Brown (Mitrovic), Notre Dame (Eskildsen), ORNL (Hermann), Sherbrooke (Taillefer), Toronto (Wei, Julian), ETH (Degiorgi), San Diego (Maple), Ames (Canfield).

Recognitions, Honors and Awards (partly attributable to support under this FWP:
Laureate SPIE Technology Achievement Award
Member The International Advisory Board, Yugoslav Materials Research Society
Chair SPIE Conference on Strongly Correlated Electron Materials, San Diego, California
Member The Program Committee, Oxide Nanocomposites Symposium, Tenerife, Spain
Co-Chair Oxide nanostructures Symposium, ICCE-11, Hilton Head, South Carolina
25 invited talks at conferences in 2004-5; 20 invited colloquia and seminar talks.

Personnel Commitments for FY2005 to Nearest +/- 10%:
I. Bozovic (100%), G. Logvenov (100%), V. Butko (100%), A. Gozar (100%) C. Petrovic 50%, H. Isaacs (100%), R. Hu (student) 100%, R. Huang (student) 100%.

Authorized Budget (BA): FY05 BA $ 1,768,337.
FY03 BA - $416K **FY04BA** - $571K **FY05BA** - $1,768K

Laboratory Name: Brookhaven National Laboratory
B&R Code: KC020201

FWP and possible subtask under FWP: Neutron Scattering

FWP Number: PO-010

Program Scope: Elastic and inelastic neutron scattering are used to investigate phenomena such as high-temperature superconductivity, charge and spin ordering in doped Mott insulators, low-dimensional and quantum-disordered antiferromagnism, and ferroelectricity. Experiments utilize national and international neutron facilities, especially instrumentation developed and supported by BNL, and single-crystal samples grown at BNL.

Major Program Achievements (over duration of support):
High-Temperature Superconductivity: Discovery and characterization of magnetic order and fluctuations in cuprates; discovery of stripe order in certain cuprates; discovery of universal magnetic spectrum for cuprates.
Doped Mott insulators: Discovery of stripe order in $La_{2-x}Sr_xNiO_{4+\delta}$ and measurement of associated spin waves; checkerboard charge plus magnetic order in $La_{0.5}Sr_{1.5}MnO_4$, $La_{1.5}Sr_{0.5}CoO_4$.
Ferroelectrics: Identification of new structural phase in $Pb(Zr_{1-x}Ti_x)O_3$; characterization of overdamped optical modes and atomic displacement pattern corresponding to polarized nano-domains in relaxor ferroelectrics.
Quantum magnetism: Characterization of dimensional crossover in systems of coupled quantum-spin chains; first observation of magnetic-field-induced order in a quantum-disordered system.
Crystal growth: Growth of very large crystals of $La_{1.875}Ba_{0.125}CuO_4$ and $Bi_2Sr_2CaCuO_{8+\delta}$ enabling detailed studies of magnetic excitations in superconductors.
Instrument development: Concept for HYSPEC at the SNS; US-Japan cold triple-axis spectrometer at HFIR

Program impact:
Results on charge-stripe correlations in cuprates have stimulated new theories of the mechanism for high-temperature superconductivity. Identification of structure and polarization direction in optimized piezoelectric $Pb(Zr_{1-x}Ti_x)O_3$ (PZT) has led to predictions of improved performance in atomically-tailored materials.

Interactions:
Internal---Condensed-Matter Physics and Materials Science Dept.: X-ray Scattering Group, Materials Synthesis and Characterization Group, Electron Spectroscopy Group, Theory Group, Superconductivity Group; Center for Functional Nanomaterials: Electron Microscopy Group
External---University of Delaware; University of Toronto, Canada; Massachusetts Institute of Technology; Johns Hopkins University; Rutgers University; Oak Ridge National Laboratory; National Institute of Standards and Technology; Institute for Solid State Physics, University of Tokyo, Japan; Institute for Materials Research, Tohoku University, Japan; Japanese Atomic Energy Research Institute; Oxford University, UK; Rutherford-Appleton Laboratory, UK; Laboratoire Léon Brillouin, France; CEA/Grenoble, France; Hahn-Meitner Institute, Berlin, Germany; Forschungszentrum Karlsruhe, Germany; Institute for Low-Temperature Physics, Ukraine

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
2 Fellows of the American Physical Society.
17 invited talks at national and international conferences in FY05.
S.M. Shapiro and I. Zaliznyak---Principle investigators of HYSPEC instrument development team
J.M. Tranquada---Divisional Associate Editor, Physical Review Letters, 2001-present; member, Lehman Review Committee for the Spallation Neutron Source; Program Advisory Committee, NIST Center for Neutron Research.

Personnel Commitments for FY2005 to Nearest +/- 10%:
J. M. Tranquada (group leader) (100%), J. Gardner (BNL/NIST Alliance, 100%), G. Gu (100%), M. Hücker (10%), L. Passell (consultant, 25%), S. M. Shapiro (83%), B. Winn (stationed at ORNL, 100%), G. Xu (100%), I. Zaliznyak (100%)

Authorized Budget (BA) for FY03, FY04, FY05: (including Neutron Instrument Development and User Support)
FY03 BA $1646K (+$675K) **FY04 BA** $1591K (+$630K) **FY05 BA** $1836K+($550K)

Laboratory Name: Brookhaven National Laboratory
B&R Code: KC0202010

FWP and possible subtask under FWP: Condensed Matter Physics--X-ray Scattering

FWP Number: PO-011

Program Scope:
The X-ray Scattering Group carries out basic studies of the structural, electronic and magnetic properties of condensed matter systems using synchrotron x-ray scattering. The Group also develops instrumentation and maintains and operates beamlines at the National Synchrotron Light Source, and at the Advanced Photon Source (APS). Particular emphasis is placed on investigation of surface and interfacial phenomena, including thin films, on electronic and magnetic structure and phase behavior, and on electronic excitations in solids. Current research is focused on strongly correlated electron systems and liquid interfaces and thin films.

Major Program Achievements (over duration of support):
The program has played a significant role in developing and applying resonant x-ray scattering techniques to the study of condensed matter systems, including especially the study of magnetic phenomena and of electronic ordering and excitations in strongly correlated systems. Highlights in FY05 include the observation of a new mode in La2-xSrxCuO4 at 500 meV with inelastic x-ray scattering, and the first observation of an “orbital speckle” pattern, using coherent soft x-ray resonant scattering. The group played a leading role in the construction, and now operation, of the Complex Materials Consortium-Collaborative Access Team (CMC-CAT) at the APS and has led the creation of a new sector dedicated to inelastic x-ray scattering (IXS-CDT), for which commissioning will begin in FY06. Efforts in the field of liquid interfaces have led to significant discoveries such as surface freezing, surface-induced layering in liquid metals and the phase behavior of Langmuir films on liquid mercury. Highlights in FY05 include the observation of ordered alkane-thiol phases on the mercury surface including the formation of long-range orientational order of the HgS2 bonds and the first measurements of the internal structure of a molecular junction between silicon and mercury.

Program impact:
The Group's longstanding programs concerned with x-ray resonant phenomena, and with liquid and soft interfaces have been seminal in stimulating related efforts worldwide, and remain among the leading programs in these areas today. Efforts in soft condensed matter led to the creation of a new FWP aimed at understanding nanotemplating phenomena. Work in inelastic x-ray scattering led, with others, to the creation of the IXS-CDT at the APS.

Interactions:
The Group typically collaborates with ~20 PIs per year, together with an approximately equal number of students and post docs. This includes significant internal BNL collaboration, both within theCondensed Matter Physics and Materials Science Dept. and more widely (in particular, the NSLS, Chemistry, and Biology Depts.) together with external collaborations with universities, other national laboratories and foreign institutions.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
22 invited talks in FY05. 2 Goldhaber Fellows, 1 Wohlfarth Award, 1 Significant Achievement in Solid State Physics, 1 Presidential Early Career Award, 3 Fellows of the APS, 1 Fellow of AAAS, 1 Brookhaven Engineering Award, 1 Brookhaven Science and Technology Award, Editorial Board Member, J. Phys. Condens. Matter..

Personnel Commitments for FY2005 to Nearest +/- 10%:
John Hill (Group Leader) (100%), Ben Ocko (75%), Jessica Thomas (100%), Stephane Grenier (100% research associate), Julian Baumert (50%), Scott Coburn (100%, Engineer), Bill Schoenig (100%, technician), Arlene Rementer (50%, secretary). Members of the Soft Matter Group (Gang, Cai, and Cheeco) are also members of the x-ray scattering group, but received no salary support from this FWP.

Authorized Budget (BA) for FY03, FY04, FY05:
FY03 BA - \$1,197K **FY04 BA -** \$1,239K **FY05 BA -** \$1,525K

Laboratory Name: Brookhaven National Laboratory
B&R Code: KC0202010 & KC 0202020

FWP and possible subtask under FWP: Materials Synthesis and Characterization

FWP Number: PO-013

Program Scope:
Synthesis and physical characterization of bulk, thin films and nanoparticles of metal oxides using ceramic and soft-chemical routes as well as various deposition techniques. Single-crystal growth using the high-temperature flux method and multi-element vapor-liquid-solid vapor transport.
Structural characterization using high-resolution synchrotron and neutron powder diffraction using X7A at the National Synchrotron Light Source as the main facility; high-pressure crystallography using diamond anvil cells; pair-distribution function (pdf) analysis of nanomaterials;

Major Program Achievements (over duration of support):
– Developed and advanced the high-pressure chemistry in zeolites and other framework structures.
– Developed novel synthesis route for family of $A_{0.3}MO_2 \times nH_2O$
– Discovered a novel family of luminescent materials
– Performed pair-distribution-functional analysis of various nanomaterials among them the structural characterization of the first room temperature electride.
– Hosted many NSLS users on X7A beamline.
– Set up laboratories for Materials Synthesis in particular single-crystal growth, sol-gel synthesis and thin film deposition techniques (SILAR).

Program impact:
Advanced the novel field of pressure-induced hydration in framework structures (i.e. zeolites, pyrochlores). A patent application entitled "Pressure-Induced Swelling in Microporous Materials" was filed.
An invention disclosure "A New Family of Luminescent Materials" was accepted.

Interactions:
Dept. of Chemical Engineering U. Delaware (D. Buttrey)
Physics Dept. Penn State University (T. Egami, W. Dmowski)
Chemistry Department University of Birmingham, UK (J.A. Hriljac)
Chemistry dept. University of Sydney, Australia (B. Kennedy)
ChevronTexaco (R Medrud, A. Bard)
Geoscience and Chemistry Dept. SUNY Stony Brook (J. Parise)
Dept. of Physics and Astronomy Michigan State University (S. Billinge, V. Petkov)
Chemistry Dept. Ohio State University (P. Woodward)

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
2004 Mineralogical Society of America Grant for Research in Crystallography (Y. Lee)
No. of Invited Talks: 4

Personnel Commitments for FY2005 to Nearest +/- 10%:
Tom Vogt (Group Leader) 100%
Yongjae Lee (postdoc on LDRD) 10%
Sangmoon Park (postdoc on LDRD) 10%
Al Langhorn (senior technical specialist) 100%
Cedomir Petrovic (50%)
Eileen Levine (33%)

Authorized Budget (BA) for FY03, FY04, FY05:

FY03 BA - $398K **FY04 BA** - $588K **FY05 BA - $**560K

Laboratory Name: Brookhaven National Laboratory
B&R Code: KC0202030

FWP and possible subtask under FWP: Theory Institute for Strongly Correlated and Complex Systems

FWP Number: PO-015

Program Scope:
To run a strong visitor program at BNL by inviting leading figures in condensed matter theory as guest scientists at the Theory Institute for Strongly Correlated and Complex Systems. The current effort is in low-dimensional strongly correlated systems, nanosystems, and complex systems and their underlying networks.

Major Program Achievements (over duration of support):
In collaboration with Prof. Chubukov we studied the single electron Green's function in d-wave superconductors. In collaboration with Dr. D. Controzzi we described the most general phase diagram of quasi-1D ladder compounds. In collaboration with Prof. A. Gogolin we developed a general theory of nanoropes.

In collaboration with Prof. K. Sneppen the computational architecture of the yeast regulatory network was studied and roles of integrators and distributors were elucidated. Together with Drs. I. Mazo and Y. Ispolatov we studied topological properties of several molecular networks operating in human cells and addressed the question of role and mechanisms of formation of homodimer proteins. Organised Workshop on Nanoscale physics in St. Petersburg; Organized Workshop on Complex Networks in Montauk, 2005.

Program Impact:
The operation of the Theory Institute strengthened the position of the Lab as one of major intellectual centers on the East Coast. It also resulted in a number of productive collaborations between visitors and BNL theorists as well as members of local experimental groups.

Interactions:
Internal: All groups in Condensed Matter Physics and Materials Science Dept., CFN, CDIC, Biology Dept., Medical Dept.
External:
Abdus Salam ETH Zurich (Prof. T. M. Rice), ICTP and SISSA, Trieste, Italy (Prof. V. Kravtsov, Dr. A. Nersesyan, D. Controzzi),
SUNY at Stony Brook (Prof. A. Abanov), University of Utah (Prof. O. Starykh)
Imperial College, London (Prof. A. Gogolin)
Niels Bohr Institute, (Prof. K. Sneppen,, A. Trusina, J. Axelsen)
Nordita, Copenhagen (Prof. P. Minhagen)
Cold Spring Harbor Laboratory (Prof. M. Chklovsky)
Ariadne Genomics (I. Mazo, Y. Ispolatov)
Univ. of Paris (Prof. B. Roehner)
Univ. of Fribourg, Switzerland (Prof. Y.-C. Zhang)
New York University (Prof. N. Rajewskii)
Columbia University (Prof. A. Rzhevsky, H. Bussemaker, A. Califano)

Recognitions, Honors and Awards (at least in some part attributable to support under this program):
None

Personnel Commitments for FY2005 to Nearest +/- 10%:
A. Abanov, V. S. Lebedev, A. O. Gogolin, A. Chubukov, N. Andrei, T. M. Rice, O. Pankratov, O. Starykh, J. Bock Axelsen, K. Eriksen, K. Sneppen, B. Roehner, Y.-C. Zhang

Authorized Budget (BA) for FY03, FY04, FY05:

FY03 BA - $159K **FY04 BA** - $346K **FY05 BA** - $400K

Laboratory Name: Brookhaven National Laboratory
B&R Code: KC0202030

FWP and possible subtask under FWP: Condensed Matter Theory
FWP Number: PO-015

Program Scope:
The emphasis of our research program is on strongly correlated electron systems (low-dimensional and frustrated magnets, disordered electrons) and on statistical mechanics of complex systems and their underlying networks. The main topics are:
- Theoretical studies of quantum and classical condensed matter systems, with extension to nano-systems.
- Understanding the evolution, statistical properties and dynamics of complex (particularly biological) systems and their underlying networks.
- Development and application of advanced non-perturbative as well as numerical (first principles) techniques in physics of strongly correlated systems.

Major Program Achievements (over duration of support):
Derivation of the universal asymptotics for finite temperature correlation functions in integrable models. This work summarizes the effort of more than 10 years. For the first time the derivation was obtained directly from the exact solution. The most general model of a gas of fermionic spin S=3/2 cold atoms is shown to be integrable and solved exactly. A tractable model of doped spin liquid is introduced and solved. This model is suggested as a prototype model for underdoped cuprates explaining the experimentally observable Fermi surface.
A systematic technique of reliably mapping out the relevant interactions in strongly correlated system is constructed based on first-principles Wannier functions. Strength of electron and lattice interactions in ordering orbitals in manganites was accurately obtained, a major step toward fundamental understanding of CMR effects. Long-standing puzzle of gapless CDW formation in dichalcogenides was explained. A model providing a unified framework for ferroelectricity and ferromagnetism was proposed and studied numerically and analytically.
The unusual network properties of homodimers (self-interacting proteins) were analyzed and explained. The effect of community structure on search and ranking in information networks was derived analytically (in the mean-field approximation) and compared to empirical data describing the hyperlink structure of the WWW network inside two US universities. The computational architecture of a biological regulatory network was studied.

Program impact: Provided many insights into behavior of strongly correlated systems and properties of complex networks.

Interactions:
Internal: All groups in Condensed Matter Physics and Material Science Dept., CFN, CDIC, Biology Dept., Medical Dept., Chemistry Dept.
External: Princeton and Columbia Universities (Prof. B. Altshuler), ETH Zurich (Prof. T. M. Rice), Harvard University (Prof. E. Demler), University of Washington, Seattle (Prof. B. Spivak) , University of Wisconsin (Prof. A. Chubukov), Abdus Salam ICTP and SISSA, Trieste, Italy (Prof. V. Kravtsov, Dr. A. Nersesyan, Dr. D. Controzzi), Imperial College, London (Prof. A. Gogolin), Argonne National Laboratory (Dr. V. Vinokur), SUNY at Stony Brook (Prof. A. Abanov), Rutgers University (Profs. A. Zamolodchikov and S. Lukyanov), Niels Bohr Institute, (Profs. K. Sneppen,, S. Krishna, J. Axelsen), Ariadne Genomics (I. Mazo, Y. Ispolatov, A. Yur'ev, E. Kotelnikova), Univ. of Paris (Profs. B. Roehner, F. Smirnov), Univ. of Fribourg, Switzerland (Prof. Y.-C. Zhang, M. Blattner), Los Alamos National Laboratory (Dr. C. Batista), New York University (Prof. N. Rajewskii), Tamkang University, Taiwan (Prof. H.-C. Hsueh), University of California, Irvine (Prof. S.R. White), University of Tennessee (A.G. Eguiluz), University of California, Davis (Prof. W.E. Pickett), University of Utah (Prof. D. Mattis), ORNL (B.C. Larson, P. Kent), LANL (C. D. Batista, J. E. Gubernatis)

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask): Alexei Tsvelik elected Fellow of the American Physical Society.
No. of invited Talks: 5 (A. Tsvelik), 7 (S. Maslov), 5 (W. Ku), 1 (R. Konik), 2 (W. Yin).

Personnel Commitments for FY2005 to Nearest +/- 10%: A.M. Tsvelik (group leader) 100%, A. Chakraborti (postdoc)100%,S. Maslov 100%, K.-K Yan (student) 100%, Wei Ku 100%, Yu. Adamov (postdoc) 100%, R. Konik 100%, D. Voljia (student) 100%, A. Chitov 100%, S. Reyes (student) 100%

Authorized Budget (BA) for FY03, FY04, FY05:

FY03 BA - $1,269K **FY04 BA** - $1,179K **FY05 BA** - $1,190K

Laboratory Name: Brookhaven National Laboratory
B&R Code: KC0202020

FWP and possible subtask under FWP: Condensed Matter Physics—Electron Spectroscopy

FWP Number: PO-016

Program Scope:
The Electron Spectroscopy Group's primary focus is on the electronic structure and dynamics of condensed matter systems. The group carries out studies on a range materials including strongly correlated systems and thin metallic films. A special emphasis is placed on studies of High Tc and related materials. The primary techniques used include High-Resolution Photoemission and Infra-Red Spectroscopy or Optical Conductivity. The experiments are carried out both within the laboratories in the Condensed Matter Physics and Materials Science Department and at the National Synchrotron Light Source. The emphasis is on the study of the low energy excitations and the nature of the interactions of the latter with their environment. The group has also established a successful pulsed laser deposition facility for the study of thin films. Future plans involve studies of nanoscale systems and will involve close collaboration and work within the newly created Center for Functional Nanomaterials.

Major Program Achievements (over duration of support):
The program has established one of the leading spectroscopy groups in the world working in the area of strongly-correlated electrons. The group has demonstrated a scaling law relating the superfluid density to the product of the normal state conductivity and the superconducting transition temperature for the high Tc superconducting cuprates, correlated the orbital dependent scattering rates observed on the Fermi surface of the ruthenate Sr_2RuO_4 with the macroscopic transport measurements. The group was also the first to identify the kink or mass renormalization observed in the nodal direction of the high Tc materials. Further the group has introduced the method of analysis in photoemission involving Momentum Didtribution Curves (MDC)

Program Impact:
Using the techniques of photoelectron spectroscopy and optical conductivity, the group has had a major impact in the areas of high Tc superconductivity, magnetic thin films and multilayers and surfaces. This is evidenced by the large number of citations and by the number of invited talks at major international and national conferences.

Interactions:
The Group collaborated with approximately sixty faculty, together with associated students and post docs. This includes significant internal BNL collaboration, both within Condensed Matter Physics and Materials Science Dept. and more widely (in particular, the NSLS, and CFN) together with external collaborations with universities, other national laboratories and foreign institutions.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
<u>Previously</u>
2 Fellows of the APS
1 Fellow of the Institute of Physics, U.K.
2001 Brookhaven Science and technology Award
No. of Invited Talks: 9 in FY04

Personnel Commitments for FY2005 to Nearest +/-10%:
Peter D. Johnson (Group Leader, 50%)
Christopher Homes (100%)
Tonica Valla (100%)
Weidong Si (100%)
Sasa Dordevic (30%-Research Associate)
Tim Kidd (75%-Research Associate)

Authorized Budget (BA) for FY03, FY04, FY05:
FY03 BA - $1,683K **FY04 BA -** $1,517K **FY05 BA -** $1,656K

Laboratory Name: Brookhaven National Laboratory
B&R Code: KC0203010

FWP and possible subtask under FWP: Condensed Matter Physics and Materials Science—Soft Matter
FWP Number: PO-034

Program Scope: The soft-matter and biomolecular materials effort is a joint project initiated by researchers in the Condensed Matter Physics and Materials Science and National Synchrotron Light Source Departments, and by several university collaborators. The primary goal of the program is to investigate the nanoscale confinement and assembly in soft matter, liquids and biomaterials through the use of patterned templates. We are investigating how templates, having well defined nanoscale chemical or surface height structures, modify the structure, phase behavior, and nucleation of liquids, liquid crystals, proteins, and biomaterials, thereby extending the current descriptions of liquid, liquid crystalline, and bulk soft-matter and biomaterial phases to the nanoscale. New methods for creating large scale templated surfaces are being developed which may have potential applications in sensors and photonic devices

Major Program Achievements:

- Development of a new chemical patterning technology, Electro Pen Nanolithography. In a single sweep of the pen, organic "ink" molecules are transferred from the tip to regions which have been oxidized by the same conducting tip (JACS, 2005)
- First verification of the shape and size dependence of wetting on chemically nanopatterned (50-300 nm) surfaces (PRL, submitted)
- Identified the wetting behavior of an organic liquids on a physically patterned surface composed of an array of nanocavities using x-ray scattering methods (PRL, 2005)
- Detailed real time GISAXS studies of selective solvent induced surface reconstruction of diblock copolymers containing salts. These studies shows the important role of salts in the development of long-range order (in collaboration with the Univ. of Mass.)
- Discovered two competing routes to Mg-calcite morphogenesis at self assembled monolayers (Crystal Growth and Design, accepted)
- Identified chiral additives to stabilize intermediate antiferroelectric smectic phases for use in device applications (Europhysics Letters, 2005)
- Demonstrated technique for in-plane nanopatterning of nematic liquid crystals that can be extended to smectics (Appl. Phys, accepted)
- Princeton /Roper CCD x-ray detector is now operational at X22B for GISAXS studies

Program Impact: The Groups work has clearly demonstrated the important role that nanopatterned surfaces can play in modifying the behavior of liquid, liquid crystal and polymer films. The nanowetting work shows the influence of Van Der Waals interactions on the shape and height of nanoliquids and confirms a long-standing theoretical prediction. The work on Electro Pen Nanolithography provides a new means of preparing chemically patterned surfaces and has received much attention and a patent application was submitted. The proposed program on "Biology-inspired programmable assembly of functional nano-structures" is an outgrowth of this program. The biomineralization and GISAXS efforts have led to NSLS workshops.

Interactions: This is a joint project among researchers in three BNL departments: Condensed Matter Physics and Materials Science, the National Synchrotron Light Source, and the Center for Functional Nanomaterials. The group collaborates with researchers at the University of Massachusetts-Amherst, Harvard University, Hebrew University, Columbia University and Case Western Reserve University.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP/subtask):
Invited Talks 8**,** Antonio Checco received the Pierre Favard 2005 award for the best PhD thesis in Microscopy between 2002-2005. This award is given by the French Society of Microscopy. Jeanette Muniz, a high school student, received the second place award in the National Junior Science and Humanities Symposium and was a semi finalist in the Intel Science Search Competition. Brookhaven Science and Technology Award – B. Ocko. Two earlier Fellows of the APS.

Personnel Commitments for FY2005: Ben Ocko (25%), Oleg Gang (50%), Ron Pindak (20%), Kyle Alvine (Harvard Univ Student) (50%), Lin Yang (10%), Univ. Mass Student (100%), Elaine DiMasi (10%), Ishtique Syed (CWRU Student) (50%), Karthik Subburaman, SBU student (50%), Yuguang Cai (100%), Brandon Chapman (100%), Antonio Checco (100%), Masa Fukuto (100%), Julian Baumert (50%)

Authorized Budget (BA): FY03, FY04, FY05:
FY 03BA - $675K **FY04 BA -** $635K **FY05 BA -** $690K

Laboratory Name: Brookhaven National Laboratory
B&R Code: KC0202020

FWP and possible subtask under FWP: Atomistic Transport Mechanisms in Revisible Complex Metal Hydrides

FWP Number: BO-130

Program Scope:

This research program has two major objectives: i) the development of a comprehensive, quantitative understanding of the fundamental, atomic-scale mechanisms underlying the facile reversible hydrogen storage in titanium-doped sodium aluminum hydride ($NaAlH_4$), the only complex hydride allowing reversible hydrogen storage known to date; and ii) the utilization of this basic knowledge for the rational screening for novel complex hydride storage materials with properties –superior to those of $NaAlH_4$. While previous research has often employed bulk compounds with complex reaction pathways and microstructures, the present program is based strongly on the use of well-defined model systems and a suite of state-of-the-art surface experiments to achieve a quantitative understanding of the important reaction mechanisms. This approach will generate data on systems accessible to first-principles calculations, and will allow an unprecedented level of interaction between experiment and theory. Key questions to be addressed via combined experimental and theoretical efforts include: i) the mechanism of hydrogen dissociation on Al surface doped with Ti; ii) the identification of the predominant carrier of mass transport, and measurements of its diffusion kinetics; and iii) the detailed reaction mechanisms and their rate-limiting step as NaH and Al react to Na_3AlH_6 and $NaAlH_4$ in the presence of hydrogen.

Major Program Achievements (over duration of support):

Since the start of the project in July 2005, we have prepared Al single crystals in two independent ultrahigh-vacuum systems (LEEM and STM) for studying the interaction of clean and Ti-doped Al surfaces with H_2 and atomic-H. First atomic-resolution STM imaging has been performed on Al(111) exposed to atomic-H. Theoretical calculations have focused on identifying pathways toward H_2 dissociation at specific Al-Ti surface complexes. The energetics of Al with near-surface Ti species was investigated, with the goal of establishing the equilibrium structure of Ti-doped Al surfaces, and hence the availability of potential active sites for dissociative H_2 adsorption. One active Al:Ti complex has been identified on Al(100). The synthesis and solid-state chemistry effort has focused on determining the structure and the dissociation kinetics of different phases of bulk AlH_3. These efforts will connect directly with the surface experiments and theory, since AlH_3 molecules and higher oligomers are anticipated to play a key role in the mass transport during cycling of $NaAlH_4$.

Program impact:

The impact of this project will be to provide a fundamental understanding of the atomic processes leading to the reversible storage of H_2 in these complex metal hydrides. This understanding will provide the basis for the development of new higher performance H_2 storage materials.

Interactions:

Yves Chabal, Rutgers University, BNL-CFN, BNL Chemistry and BNL Materials Science & Condensed Matter Physics

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
None – new program

Personnel Commitments for FY2005 to Nearest +/- 10%:
P. Sutter (10%), Muckerman (13%), S. Chaudhuri (100%), J. Graetz (75%), Y. Chabal (Contract)

Authorized Budget (BA): FY03, FY04, FY05:

FY03 BA - \$N/A **FY04 BA** - \$N/A **FY05 BA -** \$700K

Laboratory Name: Brookhaven National Laboratory
B&R Code: KC0201030

FWP and possible subtask under FWP: Reactivity of Strained Films and Interfaces – Linking adsorption/ reactivity and structure

FWP Number: AS-015-MSC

Program Scope:

It has been long recognized that the reactivity of surfaces can depend on details of atomic structure. For example, catalytic activity of transition metals can be modified by relatively small surface strains. It is also known that chemical reactions often change the structure of surfaces. For example, chemisorption will often completely redistribute atomic steps on a surface. The purpose of this proposal is to examine this complex interrelationship between surface structure and chemical reactivity in the case of thin films. At the heart of our work will be the new low energy electron microscope - x-ray photoeletron microscope (LEEM/XPEEM) that is being developed jointly between the National Synchrotron Light Source (NSLS) and the Center for Functional Nanomaterials (CFN) at Brookhaven National Laboratory. LEEM allows the imaging of the structural changes in real time, while XPEEM can monitor chemical changes with spatial resolution. This combination will allow us to correlate, in a quantitative way, the structural changes with the chemical state of the surface. For example, we will be able to correlate previously observed changes in dislocation structure with changes in the chemical state of the surface. In combination with STM, this quantitative information will supply information needed to develop atomic models of the processes involved. The ultimate goal of our work is to develop a predictive ability that will allow tailoring of interfaces for specific chemical behavior and structural behavior.

Major Program Achievements (over duration of support):

Using real-time low-energy electron microscopy, the initial nucleation and growth of RuO_2 during exposure of Ru(0001) to atomic oxygen dosed from a NO_2 gas source. RuO_2/Ru(0001) is an important low-temperature oxidation catalyst, and has recently been identified as a key model system illustrating the rational basis for the perceived "pressure gap" in catalysis: the catalytically active phase, rutile RuO_2, typically forms under conditions with high oxygen partial pressure. On the other hand, metallic Ru(0001) with chemisorbed oxygen, considered in most studies in ultrahigh vacuum (UHV), binds oxygen too strongly and is catalytically inactive. Our initial studies in this important interfacial system are aimed at understanding the oxidation mechanism of the Ru(0001) surface, its dependence on temperature, oxygen partial pressure and, importantly, on morphological features such as defects and steps of the metal surface. LEEM imaging over a range of temperatures (~600 – 800 K) revealed a surprisingly rich set of basic growth modes of ordered surface RuO_2 islands. At low temperature, surface oxidation is limited to atomic steps, and proceeds in the form of highly anisotropic, needle-like oxide islands. At higher temperatures, RuO_2 islands also nucleate on flat terraces and become gradually less elongated. The analysis of the time-dependent expansion of individual surface oxide islands suggests that fundamental aspects of the oxidation process may be temperature dependent as well.

Program impact: The capabilities developed in this FWP will have broad scientific impact in technical fields including thin film synthesis and processing, catalysis and corrosion. The impact of this work is to provide a fundamental understanding of the atomic processes of interfacial reactions.

Interactions: Norman Bartelt, Sandia National Laboratories, CA.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
Invited talks - 3

Personnel Commitments for FY2005 to Nearest +/- 10%:
R. Hwang (10%), J. Hrbek (25%), P. Sutter (25%), Bartelt (Contract)

Authorized Budget (BA): FY03, FY04, FY05:

FY03 BA - $120K	**FY04BA** - $440K	**FY05 BA -** $422K